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Thermodynamics of Combustion in a Confined Explosion

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*Thermodynamics of Combustion in a Confined Explosion

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1. Inverse Problem

Considered here are explosions from condensed TNT charges—where the expanded detonation products gases are rich in C and CO [1]. Mixing with air causes oxidation /combustion [2], which dramatically increases the pressure in confined systems (vid. Fig. 1). We treat this as an *Inverse Problem:* infer fuel consumption from the measured pressure

$$P \equiv \bar{p}(t)/p_i \tag{1}$$

This is accomplished by a Thermodynamic analysis of the system [3]. We consider *Fuel—F* and *Air—A* at fixed composition, forming *Products—P* at equilibrium. Their thermodynamic properties are displayed in the Le Chatelier diagram (Fig. 2) using

$$W_K \equiv (pv)_K / w_{Ai} \tag{2}$$

$$U_K \equiv (u_K - u_{0K})/C_A w_{Ai} = Q_K + k_K W_K \tag{3}$$

The analysis is based on the ***Thermostatic Balance Laws*** for the system:

Mass: $$Y_F + Y_A + Y_P = 1 \tag{4}$$

Volume: $$W_F Y_F + W_A Y_A + W_P Y_P = W_S \tag{5}$$

Energy: $$U_F Y_F + U_A Y_A + U_P Y_P = U_S = U_{Si} - \kappa \tag{6}$$

augmented by ***Mixture Relations*** for the *Charge*—C (F+A) and stoichiometric *Reactants—R*

$$Z_K = Z_A + F_K(Z_F - Z_A) \qquad (Z_K = W_K, U_K \;\&\; K = C, R) \tag{7}$$

where the corresponding fuel mass fractions are: $F_C \equiv 1/(1+\sigma\lambda_C)$ and $F_R \equiv 1/(1+\sigma)$ with $\sigma \equiv$ stoichiometric air-fuel ratio and λ_C =excess oxidizer coefficient.

2. Solution

The volume of the components may be related to pressure via polytropic relations and Y_P

Polytrope: $$W_K = (w_{Ki}/w_{Ai})P^{1-1/n} \qquad \text{for } K = F, A, R, C \tag{8}$$

System: $$W_S = P \tag{9}$$

Products: $$W_P = W_R + (W_S - W_C)/Y_P \tag{10}$$

while mass conservation relation (4) implies

Fuel: $$Y_F = F_C - F_R Y_P \tag{11}$$

Air: $$Y_A = (1 - F_C) - (1 - F_R) Y_P \tag{12}$$

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Next, the energy conservation relation (6) may be solved for Y_P; then by means of (3), the U_K are eliminated in favor of W_K, yielding:

$$Y_P(W_K) = \frac{k_C(W_C - W_{Ci}) + k_P(W_S - W_C) + \kappa}{|Q_P - Q_R| - (k_P - k_R)W_R} \tag{13}$$

Finally (8)-(10) are used to replace W_K by P, thereby expressing the Products mass fraction

$$Y_P(P) = \frac{k_P P - (k_P - k_C)P^{1-1/n} - k_C + \kappa}{|Q_P - Q_R| - (k_P - k_R)P^{1-1/n}} \tag{14}$$

in terms of pressure and the thermodynamic properties of the components.

3. Application

The solution for TNT may be evaluated from the properties of Fig. 2: $k_P = 1.706$, $k_R = 1.20$, $k_C = k_A = 1$, $Q_P = -11.63$, $Q_R = -3.63$, $n = 1.38$, $F_C = 0.05$, $F_R = 0.238$, $C_A = 2.59$ and $w_{Ai} = 128\ J/g$. Thus, the mass-fraction of fuel consumed by combustion becomes

$$x_F(P) \equiv \frac{F_R}{F_C} Y_P = 4.76 \frac{1.706P - 0.706P^{0.275} - 1 + \kappa}{8.00 - 0.506P^{0.275}} \tag{15}$$

The experimental pressure history (Fig. 1) was fit by

$$P(t) = 2 - e^{-t/4.42ms} \tag{16}$$

where $p_i = 1.92 \pm 0.1$bars, $p_f = 3.80 \pm 0.1$ bars and $P_f = p_f/p_i = 1.98$. It may be used to eliminate P in favor of time—thereby establishing the temporal solution. The results are displayed in Figs. 3—6 for the case of adiabatic walls ($\kappa = 0$).

4. Conclusions

The Model expounded here represents a valuable tool for extracting the evolution of combustion system from a readily measurable quantity (pressure). The Model establishes the fuel consumption history as well as the evolution of thermodynamic solution (specific volumes, energies and densities) of the components that will generate the observed pressure profile. This solution in Thermodynamic (State) Space provides extraordinarily clear insight into the combustion process, which is normally clouded by a myriad of transport processes that occur in physical space.

References

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